

Amendments to the Claims:

This listing of claims will replace all prior versions, and listings, of claims in the application:

Listing of Claims:

1. (currently amended) A method of drug discovery and development comprising:
 - providing a full-rank database of interactions between a plurality of molecular targets and a plurality of compounds, wherein the database comprises a set of descriptors that describe structural features of the molecular targets and the compounds;
 - selecting two or more molecular targets that are associated with a disease state for which the drug discovery and development are directed;
 - analyzing the database to identify a set of compound descriptors associated with a set of desired interactions with the two or more molecular targets;
 - selecting a plurality of candidate compounds as potential drugs to treat the disease state;
 - representing each of the candidate compounds in terms of the descriptors;
 - identifying the candidate compounds having the set of compound descriptors associated with the set of desired interactions; and
 - providing output specifying the identified candidate compounds.
2. (previously presented) The method of claim 1, wherein the plurality of candidate compounds comprise known compounds.
3. (currently amended) The method of claim 1, wherein the analyzing step comprises recursive partitioning.
4. (previously presented) The method of claim 1, wherein the descriptors comprise 2-D bond length descriptors.

5. (currently amended) A method of drug discovery and development comprising:

providing a full-rank database of interactions between a plurality of molecular targets and a plurality of compounds, wherein the database comprises a set of descriptors that describe structural features of the molecular targets and the compounds;

analyzing the database to identify a set of compound descriptors associated with both (a) a desired activity at one or more molecular targets that are associated with a disease state for which the drug discovery and development are directed and (b) the absence of an undesired activity at one or more molecular targets that are associated with undesired therapeutic effects;

representing a drug candidate in terms of the descriptors;

determining whether the drug candidate contains the set of compound descriptors;

and

providing output based on the determination, the output specifying whether the drug candidate does or does not contain the set of compound descriptors.

6. (previously presented) The method of claim 5, wherein the drug candidate is a known compound.

7. (currently amended) The method of claim 5, wherein there are multiple targets associated with the disease state.

8. (original) The method of claim 5, wherein the undesired therapeutic effect is a side effect.

9–37 (canceled)

38. (previously presented) The method of claim 5, wherein the undesired therapeutic effect is toxicity.

39. (canceled)

40. (previously presented) The method of claim 5, wherein the descriptors comprise 2-D bond length descriptors.

41. (currently amended) The method of claim 5, wherein the analyzing step comprises recursive partitioning.